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Average Structures of a Single Knotted Ring Polymer

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ブラウン動力学シミュレーション法を用いて結び目をもつ孤立環状高分子の良溶媒中の平均構造を調べた研究 (J. Phys. Soc. Jpn. **77** (2008) No. 12) の結果について紹介する. 平均構造は, シミュレーションで得た個々の構造を平均構造からの二乗変位が最小となるように回転・並進させた後, それらを平均した構造として反復法で得られる. 三葉結び目をもつ環状高分子の平均構造を評価した結果, 各平均構造の結び目部分は, 鎖長が短いときには非局在状態にあるが, 鎖長が長くなると局在化することがわかった.

The results of a Brownian dynamics study on average structures of a knotted ring polymer in good solvent (J. Phys. Soc. Jpn. **77** (2008) No. 12) are presented. The average structure is self-consistently calculated as the average of conformation vectors obtained from a simulation each of which is translated and rotated to minimize its distance from the average of the conformation vectors. In the estimated average structures of single ring polymers with the trefoil knot, the knotted part of each average structure is delocalized for small values of the number of segments N and becomes localized as N increases.

1 Introduction

The topological effects caused by the entanglement of polymers on the properties of polymer systems have attracted much interest.[1] A single knotted ring polymer is one of the self-entangled systems and can be considered as an ideal system for the study of topological effects. An unresolved important problem in a single knotted ring polymer is the dependence of topological effects of the knot on the polymer length. In the following, we present the results of a study[2] which confirms the localization of the knotted part of a single knotted ring polymer in good solvent by directly observing its average structure (AS) in three dimensions through Brownian dynamics simulations. The AS is self-consistently calculated as the average of conformation vectors obtained from a simulation each of which is translated and rotated to minimize its distance from the average of the conformation vectors. The AS has been frequently used in simulation studies of biopolymers, which are typically heteropolymers. In contrast, a ring polymer considered here is a homopolymer and has the translational symmetry along the polymer chain. An extension of the definition of the AS is proposed by utilizing the translational symmetry.

2 Model and Average Structure

Brownian dynamics simulations of a knotted ring polymer in good solvent are performed by using a bead-spring model. The dynamics of the i th segment of a single ring polymer with N segments is described by the overdamped Langevin equation for the position of the i th segment with Gaussian white random forces.

The AS is estimated by using conformations of a polymer sampled in simulations. Let $\mathbf{R}_i(m)$ denote the position of the i th segment relative to the center of mass of the polymer in the m th sample. Then, a $3N$ -dimensional conformation vector $\mathbf{C}(m) = {}^t(\mathbf{R}_1(m), \mathbf{R}_2(m), \dots, \mathbf{R}_N(m))$ represents a structure of the polymer in the m th sample. From each $\mathbf{C}(m)$, $2N$ conformations, $\tilde{\mathbf{C}}(m, 1), \dots, \tilde{\mathbf{C}}(m, 2N)$, can be generated by changing the numbering of the segments as follows: $\tilde{\mathbf{C}}(m, k) = {}^t(\mathbf{R}_{n(1,k)}(m), \mathbf{R}_{n(2,k)}(m), \dots, \mathbf{R}_{n(N,k)}(m))$, where $n(i, k) = (1 - 2r)i_j + r(N + 1)$ with $i_j = ((i + j - 1) \bmod N) + 1$, $j = \lfloor (k - 1)/2 \rfloor$, and $r = (k - 1) \bmod 2 = k - 1 - 2j$. For each $\tilde{\mathbf{C}}(m, k)$, a three-dimensional rotation $\mathcal{R}_{m,k}$, which minimizes the square distance $d^2(m, k)$

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between the rotated conformation vector $\mathcal{R}_{m,k}(\tilde{\mathbf{C}}(m,k))$ and the average conformation vector \mathbf{C}^{av} , is determined.[3] Here,

$$d^2(m,k) = \left(\mathcal{R}_{m,k}(\tilde{\mathbf{C}}(m,k)) - \mathbf{C}^{\text{av}} \right)^2 = \sum_{i=1}^N \left(\mathcal{R}_{m,k}(\mathbf{R}_{n(i,k)}(m)) - \mathbf{R}_i^{\text{av}} \right)^2. \quad (1)$$

Thus, the conformation $\tilde{\mathbf{C}}(m,k)$ is fitted to the average conformation \mathbf{C}^{av} by the rotation $\mathcal{R}_{m,k}$. The conformation vectors $\tilde{\mathbf{C}}(m,k)$ with $k = 1, \dots, 2N$ are considered to represent the same structure as $\mathbf{C}(m)$, because all the segments of a homopolymer are equivalent. Therefore, the best fit of a sampled conformation $\mathbf{C}(m)$ to the average conformation is given by the rotated conformation $\mathcal{R}_{m,k_{\min}(m)}(\tilde{\mathbf{C}}(m,k_{\min}(m)))$, where $k_{\min}(m)$ is the value of k that gives the smallest value of $d^2(m,k)$ with m fixed. The average of the best fitted conformations gives the average conformation vector \mathbf{C}^{av} as

$$\mathbf{C}^{\text{av}} = \frac{1}{M} \sum_{m=1}^M \mathcal{R}_{m,k_{\min}(m)}(\tilde{\mathbf{C}}(m,k_{\min}(m))). \quad (2)$$

3 Results of Simulations

Figure 1 shows the ASs of single ring polymers with the trefoil knot. The bonds connecting adjacent segments and the center of mass of the ring polymer are represented by the cylinders and spheres, respectively. The knot type of the ASs is the same as that of the original conformations for each N . The knotted part is delocalized for small values of N and is localized for large values of N . The crossover from the delocalized state, where the center of mass is inside of the knotted part, to the localized state, where the center of mass is outside of the knotted part, occurs around the segment number $N_x \simeq 120$, which is consistent with the transition segment number $N_t = 96\text{--}144$ found in the previous study on the relaxation rates of single ring polymers.[4]

4 Conclusion

In the case of single ring polymers with the trefoil knot, the knotted part of the ASs is expanded along the entire structure for small values of N and localized to a part of the structure for large values of N . The crossover from the delocalized state to the localized state occurs around the crossover segment number $N_x \simeq 120$ and provides strong evidence for the localization of the knotted part.

References

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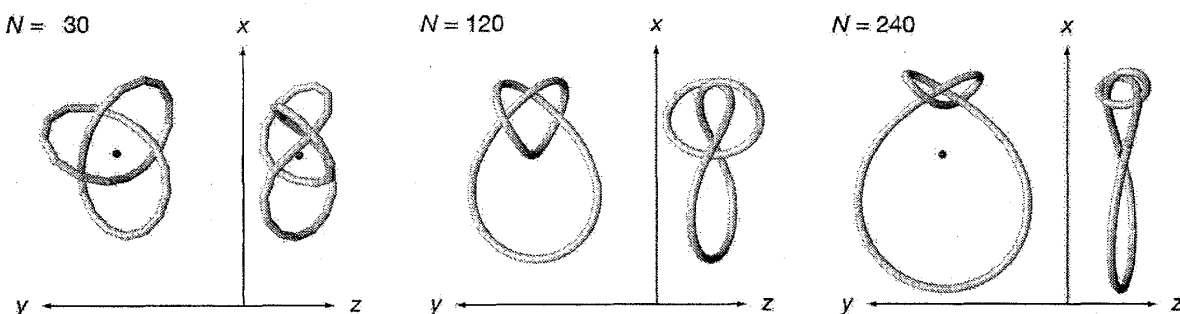


Figure 1: ASs of single ring polymers with the trefoil knot.[2]